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1 Methodologies to assess mean annual air pollution concentration combining 2 numerical results and wind roses

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15

16 ABSTRACT

Numerical models are valuable tools to assess air pollutant concentrations in cities which can 17 18 be used to define new strategies to achieve sustainable cities of the future in terms of air quality. Numerical results are however difficult to be directly compared to air quality standards since 19 they are usually valid only for specific wind speed and direction while some standards are on 20 annual values. The purpose of this paper is to present existing and new methodologies to turn 21 22 numerical results into mean annual concentrations and discuss their limitations. To this end, 23 methodologies to assess wind speed distribution based on wind rose data are presented first. 24 Then, methodologies are compared to assess mean annual concentrations based on numerical 25 results and on wind speed distributions. According to the results, a Weibull distribution can be used to accurately assess wind speed distribution in France, but the results can be improved 26 27 using a sigmoid function presented in this paper. It is also shown that using the wind rose data directly to assess mean annual concentrations can lead to underestimations of annual 28 29 concentrations. Finally, the limitations of discrete methodologies to assess mean annual 30 concentrations are discussed and a new methodology using continuous functions is described.

31

32 **1. Introduction**

33 Over the past decades, outdoor air pollution has become a major issue, especially in highly 34 densified urban areas where pollutant sources are numerous and air pollutant emissions high. 35 In order to protect people from excessive exposure to air pollution, which can cause several 36 diseases (Anderson et al., 2012; Kim et al., 2015), the World Health Organization (WHO) have 37 recommended standard values that must not be exceeded for different pollutants such as 38 nitrogen dioxide (NO₂) and particulate matter (EU, 2008; WHO, 2017) to protect population health, and the European Union (EU) decided to respect the same or other standards depending 39 40 on the air pollutants. Among the different types of values given as standards, studies have shown that annual standards are generally more constraining and harder to reach than the other 41 42 standards (Chaloulakou et al., 2008; Jenkin, 2004).

In the meantime, recent studies have shown that the indoor air quality is strongly correlated with the outdoor one: while for nitrogen dioxide a 5% increase in indoor air pollutant concentrations can be expected for only a 1% increase in outdoor concentrations (Shaw et al., 2020), for particulate matters such as PM_{2.5} the outdoor concentration can contribute from 27% to 65% of the indoor concentration (Bai et al., 2020). Being able to assess outdoor pollutant concentrations is therefore a necessity to improve air quality in the outdoor built environment, but also in the indoor one (Ścibor et al., 2019).

Annual concentrations can be assessed using both on-site monitoring and numerical modeling. On site monitoring requires measurements over long periods to be able to assess mean annual concentrations of pollutants, although a recent study has shown that mean annual concentration of NO_2 can be assessed using only one month of data (Jurado et al., 2020), which significantly reduces the measurement time required. Monitoring nonetheless has other limitations: it does not allow assessing the future evolution of the built environment or pollutant emissions, thus, 56 limiting its applicability to achieve the smart sustainable cities of the future as defined by Bibri 57 and Krogstie (2017). Numerical modelling can overcome these limitations and can help define 58 new strategies to improve air quality in cities combining wind data, various air pollution 59 scenarios and urban morphologies (Yang et al., 2020). Among the several models currently 60 available, Computational Fluid Dynamics (CFD) has shown great potential for modeling pollutant dispersion from traffic-induced emissions by including numerous physical 61 62 phenomena such as the effects of trees (Buccolieri et al., 2018; Santiago et al., 2019; Vranckx et al., 2015) and heat exchanges (Qu et al., 2012; Toparlar et al., 2017; Wang et al., 2011) on 63 the scale of a neighborhood. However, this type of numerical result cannot be directly compared 64 with the annual standards. Methodologies designed to assess mean annual concentrations based 65 on numerical results, such as described by Solazzo et al. (2011), are thus required and further 66 work is required to improve these methodologies and assess their limits. 67

The aim of this study is to provide tools and methodologies to assess mean annual 68 concentrations based on numerical results and wind rose data to improve air quality in built 69 70 environment and cities. It is firstly to evaluate whether it is possible to assess continuous wind 71 speed distributions based on wind rose data. To do so, a statistical law called Weibull distribution is compared with a new sigmoid-based function built for the purpose of this study. 72 73 Secondly, it is to present and compare a discrete methodology usually used to assess mean 74 annual concentrations based on numerical results with a continuous methodology built for the 75 purpose of this study, and to discuss their respective advantages and limitations. The data used 76 for the wind speed distribution assessments, the area modeled and the CFD model used for 77 illustration purposes are presented in Section 2. Then, the description and the comparison of 78 the different methodologies are presented in Section 3 and, finally, a discussion is provided in 79 Section 4.

80

81

82 **2. Material and methods**

83 2.1. Meteorological data

84 2.1.1. Data location

This work uses wind velocity and wind direction data from four cities in France. These cities were chosen to cover most of France to obtain representative results and include the cities of Strasbourg (Grand-Est region), Nîmes (Occitanie region), Brest (Bretagne region) and Lille (Hauts-de-France region). In particular, the data were obtained from the stations named Strasbourg-Entzheim, Nîmes-Courbessac, Brest-Guipavas and Lille-Lesquin, respectively. The location of these stations and their corresponding regions are presented in Fig. 1.



- 91
- 92

Fig. 1. Location of the different meteorological stations used.

93 2.1.2. Data availability and data range

The data used in this work were provided by Météo-France, a public institution and France's official meteorology and climatology service. The data are mainly couples of wind velocity and wind direction over a twenty-year period from 1999 to 2018, except for the Strasbourg97 Entzheim station where it is a ten-year period from 1999 to 2008. The data were obtained via a 98 personal request addressed to Météo-France and were not available on open-access. A summary 99 of the information of the stations is presented in Table 1, with the time ranges of the data and 100 the number of data available (the coordinates are given in the World Geodetic System 1984).

101 Table 1. Summary of the available data.

102

	Data availability					
Location	Latitude	Longitude	Altitude	Time range	Number of valid cases	Number of missing cases
Brest - Guipavas	48°27'00''N	4°22'59"O	94 m	2009 - 2018	29,171	45
Lille - Lesquin	50°34'12''N	3°05'51"E	47 m	2009 - 2018	29,185	31
Nîmes - Courbessac	43°51'24"N	4°24'22''E	59 m	2009 - 2018	29,214	2
Strasbourg - Entzheim	48°32'58"N	7°38'25"E	150 m	1999 - 2008	29,199	25
	<u>.</u>	Į.				

103 All the data were monitored from wind sensors placed 10 meters from the ground and the wind frequencies are available for each wind direction with 20° steps for two distinct wind 104 discretizations: a "basic" discretization giving wind frequencies for 4 velocity ranges (from 0 105 to 1.5 m/s, 1.5 to 3.5 m/s, 3.5 to 8 m/s and more than 8 m/s), illustrated in Fig. 2. (A); and a 106 107 "detailed" discretization giving wind frequencies by 1 m/s steps except between 0 and 0.5 m/s, illustrated in Fig. 2. (B). The "basic" discretization is a common format mostly found in wind 108 roses (possibly with different velocity ranges) while the "detailed" data are less common and 109 110 more expensive.



Fig. 2. Example of data for Strasbourg and a 200° wind direction with (A) only 4 ranges of velocities and (B) the detailed
data discretized in 18 ranges.

The wind roses for each meteorological station considered in this work and based on the "basic" 4-velocity-range discretization described in Fig. 2. (A) are provided in Fig. 3. This figure shows how the monitoring locations considered in this study give distinct but complementary information, with for example many high velocities at Brest compared to Strasbourg and Nîmes, where almost no velocities were monitored over 8 m/s, and with dominant wind directions at Nîmes and Strasbourg compared to the other stations.





121

Fig. 3. Wind roses for each location considered.

122

123 2.1.3. Interpolation functions

124 A two-parametric continuous probability function, the Weibull distribution, mainly used in the 125 wind power industry, can be used to describe wind speed distribution (Kumar et al., 2019; Mahmood et al., 2019). The equation of the corresponding probability density function is givenin (1).

128
$$f(v) = \frac{k}{\lambda} \left(\frac{v}{\lambda}\right)^{k-1} e^{-(v/\lambda)^k}$$
(1)

129 where v is the wind velocity, k is the shape parameter and λ is the scale parameter of the 130 distribution, with k and λ being positive.

For the purpose of this study, an original 5-parametric continuous function was built to determine the "detailed" wind discretization based on the "basic" 4-velocity-range wind discretization. This function, called Sigmoid function, based on the composition of two sigmoid functions, is given in (2). The two functions will be compared in the results section.

135
$$f(v) = \alpha \cdot \left(-1 + \frac{1}{1 + \beta_1 \cdot e^{-\gamma_1 \cdot v}} + \frac{1}{1 + \beta_2 \cdot e^{\gamma_2 \cdot v}} \right)$$
(2)

136 where α , β_1 , β_2 , γ_1 and γ_2 are positive parameters.

137

138 2.2. Numerical model

Simulations were performed using the unsteady and incompressible solver *pimpleFoam* from OpenFOAM 6.0. A Reynolds-Averaged Navier-Stokes (RANS) methodology was used to solve the Navier-Stokes equations with the RNG k-ε turbulence model, and the transport of particulate matter was performed using a transport equation. This solver was validated previously in Reiminger et al. (2020).

The area chosen to illustrate the methodologies discussed in this paper is located in Schiltigheim, France (48°36'24", 7°44'00"), a few kilometers north of Strasbourg. This area, as well as the only road considered as an emission source in this study (D120, rue de la Paix), are illustrated in Fig. 4. (A). PM₁₀ traffic-related emissions were estimated at 1.39 mg/s using daily annual mean traffic and were applied along the street considering its length in the numerical
domain (200 m), its width (9 m) and an emission height of 0.5 m to take into account initial
dispersion.

151 The recommendations given by Franke et al. (2007) were followed. In particular, with H being 152 the highest building height (16 m), the distances between the buildings and the lateral 153 boundaries are at least 5H, the distances between the inlet and the buildings as well as for the 154 outlet and the buildings are at least 5H and the domain height is around 6H. An illustration of the resulting 3D sketch is presented in Fig. 4. (B). A grid sensitivity test was performed and 155 showed that hexahedral meshes of 1 m in the study area and 0.5 m near the building walls are 156 157 sufficient, leading to a more comparable resolution than other CFD studies (Blocken, 2015) and 158 leading to a total number of around 800,000 cells. The resulting mesh is illustrated in Fig. 5.



- 159
- 160 Fig. 4. Illustration of (A) the area of Strasbourg modeled with the road considered for the traffic-related emissions (white
- 161 dashed lines), and (B) the corresponding area built in 3D for the numerical simulations with the emission source (red).

162

163 No-slip conditions (U = 0 m/s) were applied to the building walls and ground, and symmetry 164 conditions to the lateral and the top boundaries. A freestream condition was applied to the outlet 165 boundary, and neutral velocity, turbulent kinetic energy and turbulent dissipation profiles 166 suggested by Richards and Norris (2011) were applied to the inlet boundary.

167 A total of 18 simulations were performed using the same wind velocity ($U_{10 m} = 1.5 \text{ m/s}$) but with different wind directions from 0° to 340° using a 20° step. Since the simulations were 168 169 performed in neutral conditions and without traffic-induced turbulence, the dimensionless concentration C^* given in (3) is a function only of the wind direction (Schatzmann and Leitl, 170 171 2011). In other words, this means that considering the previous hypothesis, and for a given emission and building configuration (leading to constant H. L/q ratio), only one simulation is 172 needed for each wind direction simulated. The pollutant concentrations for a non-simulated 173 wind velocity u can therefore be computed using (4). 174

175
$$C^* = \frac{C.U.H.L}{q}$$
(3)

176 where C^* is the dimensionless concentration, *C* is the concentration, *U* the wind velocity, *H* 177 the characteristic building height and q/L the source strength of emission.

178
$$C_u = U_{ref} \cdot \frac{C_{ref}}{u} \quad (4)$$

179 where C_u is the pollutant concentration for the wind velocity u not simulated and C_{ref} the 180 pollutant concentration for the simulated wind velocity U_{ref} .



182 Fig. 5. Illustration of the meshes in the computational domain with the emission source (red), with 0.5 m meshes near the

183

181

buildings and 1 m in the study area.

184 **3. Results**

- 185 3.1. Wind data interpolation
- 186 3.1.1. Comparison between the Weibull distribution and the sigmoid function

The best fitting parameters of the two functions were determined for the whole dataset using a 187 188 non-linear solver and the "basic" 4-velocity-range wind data. The solver was set up to solve 189 equation (5) for the four-velocity ranges $[0, 1.5[, [1.5, 4.5[, [4.5, 8[and [8, +\infty[for both the$ 190 Weibull and the sigmoid functions. This equation reflects that the sum of the frequencies 191 between two wind velocities (i.e. the area under the curve) must be equal to the frequency given 192 in the "basic" 4-velocity-range wind data. Since the sigmoid function has five parameters, a 193 fifth equation to be solved was added only for this function and corresponds to (6). With this 194 equation, it is assumed that the wind frequency tends toward 0% when the wind speed tends 195 toward 0 m/s, as for the Weibull distribution.

196
$$\int_{a}^{b} f(v) \, dv = FVR_{[a;b[}$$
(5)

197
$$f(0) = 0$$
 (6)

10/26

198 where f(v) is the Weibull or the sigmoid function and $FVR_{[a;b[}$ is the wind frequency given in 199 the 4-velocity-range data for wind velocities ranging from *a* included to *b* excluded.

Fig. 6 (A–D) shows a comparison between the Weibull distribution, the sigmoid function and the "detailed" 18-velocity-range data for one wind direction of each meteorological station. According to these figures, the two functions generally give the same trends, and both appear to give a good estimation of the "detailed" wind data. However, depending on the case, the Weibull function can provide improvements in comparison to the sigmoid function, as in Fig. 6. (A), or vice versa, the sigmoid function can provide improvements in comparison to the Weibull function, as in Fig. 6. (D).



207

Fig. 6. (A–D) Weibull distribution and sigmoid function results compared to the detailed meteorological wind frequency data for one wind direction at each station considered and (E) a notched box plot of the mean error over one wind direction with all stations included for both functions.

To better compare the two functions, a notched box plot of the mean error over one wind direction is given in Fig. 6. (E). According to this figure, the sigmoid function gives generally better results compared to the Weibull distribution, with a lower maximal error (30.0% and

214 33.1% respectively); a lower first quartile (8.1% and 9.5% resp.); a lower third quartile (13.8% 215 and 14.5% resp.); a lower mean (11.7% and 13.5% resp.); and a lower median (10.6% and 216 12.4% resp.). The differences are, however, small and may not be significant, especially for the 217 median because the notches slightly overlap. These differences between the Weibull 218 distribution and the sigmoid function are also location dependent, with for example better 219 prediction of the wind distribution in Strasbourg using the sigmoid function and an equivalent 220 prediction in Brest. Finally, it should be noted that both functions can lead to underestimations 221 of the lower wind velocity frequencies, as shown in Fig. 6. (A) and (D).

According to the previous results, the Weibull distribution and the sigmoid function can accurately reproduce the "detailed" wind distribution based on a "basic" 4-velocity-range discretization with an average error of around 12% over the four stations considered in France. They can nonetheless lead to underestimations of the low wind velocity frequencies, for which the highest pollutant concentrations appear.

227

228 3.1.2. Optimization of the sigmoid function interpolation for low wind velocities

The parametrization of the sigmoid function, called standard sigmoid function, was modified to improve the estimation of the low wind velocity frequencies in order to avoid underestimating pollutant concentrations.

Based on all the meteorological data considered in this study, it was found that the underestimation of low wind velocity frequencies occurs mostly when the frequency of the first velocity range is lower than the frequency of the second velocity range. In this specific case, the optimized sigmoid function still needs the equation (5) for the four-velocity ranges given in the "basic" wind data, but equation (6) is replaced by equation (7); otherwise, the previous parametrization using equations (5) and (6) is kept.

238
$$f(0) = FVR_{[0;\alpha[}\frac{FVR_{[0,\alpha[}}{FVR_{[\alpha,\beta[}}$$
(7)

where $FVR_{[0,\alpha[}$ is the wind frequency for the first range of velocities given in the 4-velocityrange data and $FVR_{[\alpha,\beta[}$ is the wind frequency for the second range of velocities (e.g., in this study $\alpha = 1.5$ and $\beta = 4.5$).

242 The methodology for the optimized sigmoid function is illustrated in Fig. 7. (A–B): when the 243 frequency of the first velocity range is higher than the second, as in Fig. 7. (A1), the standard parametrization of the sigmoid function can be used because the low wind velocity frequencies 244 are estimated accurately, as in Fig. 7. (A2), when the frequency of the first velocity range is 245 lower than the second, as in Fig. 7. (B1), the standard parametrization leads to underestimations 246 of low wind velocity frequencies and the optimized parametrization should be used instead, 247 leading to a better estimation of the frequencies, as shown by the blue curve in Fig. 7. (B2) 248 249 compared to the red curve.





Fig. 7. (A–B) Illustration of the optimized sigmoid function methodology and (C) comparison with the standard sigmoid function results.

253 The improvements with the optimized sigmoid function compared to the standard function were 254 assessed and the results are presented in Fig. 7. (C). For this comparison, only the wind 255 directions where the optimized function was applied are considered and the errors compared to 256 the "detailed" 18-velocity-range data were calculated for the low wind velocity frequencies 257 (between 0 and 3.5 m/s). According to this figure, the optimized sigmoid function gives 258 improvements over the standard sigmoid function with a lower maximal error (41.0% and 259 44.4% respectively); a lower first quartile (9.2% and 12.9% resp.); a lower third quartile (22.4% 260 and 25.5% resp.); a lower mean error (15.2% and 19.4% resp.); and a lower median (13.0% and 19.6% resp.). The improvements using the optimized function are significative, in particular for 261 the median since the box plot notches do not overlap; they are also location dependent. A global 262 263 improvement of the wind distribution prediction ranging between 20% and 45% is observed in Strasbourg, Lille and Nîmes while no improvement is observed in Brest. 264

According to the previous results, using the optimized sigmoid function can improve the reproduction of the "detailed" wind distribution based on a "basic" 4-velocity-range compared to the standard sigmoid function, especially for low wind velocities.

268 3.2. Mean annual concentration assessment

269 3.2.1. Discrete methodology with intermediate velocities

Initially, mean annual concentrations based on the CFD results can be calculated using a discrete methodology. This methodology considers that the mean annual concentration at a given location is composed of several small contributions of different wind velocities and wind directions. The mean concentration over one wind direction can be calculated with equation (8) and the mean annual concentration with equation (9). A similar methodology can be found in (Solazzo et al., 2011).

276
$$\bar{C}_{d} = \frac{\sum_{r=1}^{n} C_{d,r} \cdot f_{d,r}}{\sum_{r=1}^{n} f_{d,r}} + C_{bg} \quad (8)$$

277
$$\bar{C} = \frac{\sum_{i=1}^{n} \bar{C}_{d} \cdot f_{d}}{\sum_{i=1}^{n} f_{d}} \quad (9)$$

where \bar{C}_d is the mean concentration over one wind direction, $C_{d,r}$ is the concentration for a given wind direction *d* and a given wind velocity range *r*, $f_{d,r}$ is the frequency for a given wind direction and a given wind velocity range, C_{bg} is the background concentration, \bar{C} is the mean annual concentration and f_d the total frequency of a given wind direction.

With this methodology, it is necessary to choose a wind velocity in each velocity range for which the concentration will be calculated based on the CFD result. A simple choice is to consider an intermediate velocity, noted v_i , corresponding to the average between the minimal and the maximal value of the velocity range (e.g., for the velocity range [1.5, 4.5], the intermediate value is 3 m/s).

A comparison of results for this methodology is given in Fig. 8. with distinct cases considering (A) the "basic" 4-velocity-range frequencies, (B) the "detailed" 18-velocity-range frequencies, (C) the frequencies calculated with the sigmoid function, and (D) the frequencies calculated with the optimized sigmoid function. No background concentration is considered in this study to permit better comparison of the results.



292

Fig. 8. Mean annual concentrations without background concentration based on (A) the "basic" 4-velocity-range monitoring
data, (B) the "detailed" 18-velocity-range monitoring data, (C) the sigmoid interpolation data and (D) the optimized sigmoid
interpolation data.

296 Initially, it can be seen that using the "basic" 4-velocity-range data leads to an underestimation 297 of the concentrations compared to the case using "detailed" 18-velocity-range data by around 19%. When calculating the "detailed" wind velocity distribution based on the "basic" data with 298 299 the sigmoid function, the difference is reduced to 12.9%. Finally, the best results are obtained 300 when using the optimized sigmoid function with an underestimation of 3.4%. According to these results, using the "basic" 4-velocity-range frequencies can give an estimation of the mean 301 302 annual concentrations but is not sufficient to reach good accuracy compared to the mean annual 303 concentration calculated with the "detailed" wind velocity distribution. However, using the 304 sigmoid function and especially the optimized variant significatively improves the results, leading to almost the same results as those obtained with the "detailed" wind velocitydistribution.

307 *3.2.2. Discrete methodology with representative velocities*

308 The previous methodology used to compute annual concentrations, which was easy to set up, 309 nonetheless has certain weaknesses that mostly concern the choice of the wind velocity for 310 which the concentrations will be calculated, based on the CFD results. Using an intermediate 311 velocity v_i corresponding to the average between the minimal and the maximal value of the 312 velocity range can lead to underestimations of the mean annual concentrations. Indeed, in doing so, it is implicitly assumed that the concentration is constant with the wind velocity in a given 313 314 wind velocity range. However, according to equation (4), this assumption is wrong because the 315 concentration evolves hyperbolically with velocity. The representative velocity over one 316 velocity range, considering the hyperbolic evolution of the concentration, is given in (11) as a 317 result of (10) and (4).

318
$$\frac{1}{2} \int_{v_{min}}^{v_{max}} c(v) \, dv = \int_{v_{min}}^{v_r} c(v) \, dv \quad (10)$$

319
$$v_r = \sqrt{\frac{2}{\frac{1}{v_{max}^2} + \frac{1}{v_{min}^2}}} \quad (11)$$

where v_{max} and v_{min} are respectively the maximal and the minimal velocities of the velocity range, v_r is the representative velocity of the velocity range and c(v) the equation describing the evolution of the concentration as a function of the wind velocity, i.e. equation (4).

323 The representative velocities v_r were calculated with equation (11) and compared to the 324 intermediate velocities v_i . It is noteworthy that for a velocity range with a minimal velocity of 325 0 m/s, it is mathematically not possible to compute the representative velocity due to the domain definition of the function. A choice is therefore required; for the purpose of this study, the same ratio v_r/v_i as for [0.5, 1.5] was considered.

According to the results summarized in Table 2. for wind velocities ranging from 0 to 6.5 m/s, the intermediate velocity can be much higher than the representative velocity for low velocities. For example, for wind velocities ranging from 0.5 to 1.5 m/s, the intermediate velocity of 1 m/s is almost twice as high as the representative velocity of 0.67 m/s. For higher velocity ranges, such as [2.5, 3.5] or more, the differences can be neglected. This last statement is true for 1 m/s steps between the minimal and the maximal velocities of the velocity range but can become

334 wrong for higher velocity steps.

335

Table 2. Comparison between the intermediate velocity v_i and the representative velocity v_r (*: the representative velocity was calculated considering the same ratio v_r/v_i as for [0.5, 1.5]).

v _{min} [m/s]	0	0.5	1.5	2.5	3.5	4.5	5.5
v_{max} [m/s]	0.5	1.5	2.5	3.5	4.5	5.5	6.5
$v_i [\text{m/s}]$	0.25	1.00	2.00	3.00	4.00	5.00	6.00
$v_r \text{ [m/s]}$	0.1675*	0.67	1.82	2.88	3.90	4.92	5.94
v_r/v_i	0.67*	0.67	0.91	0.96	0.97	0.98	0.99

338

339 Fig. 9. shows a comparison of the mean annual concentrations when using the intermediate velocity and when using the representative velocity, based on the "detailed" 18-velocity-range 340 341 wind distribution. According to the results, using the intermediate velocity leads to considerable 342 underestimations of the mean annual concentrations compared to the use of the representative 343 velocity. The underestimation is about 20%. When using the discrete methodology presented 344 in Section 3.2.1., it is therefore suggested to use the representative velocity instead of the 345 intermediate velocity to better take into account the hyperbolic evolution of the pollutant 346 concentrations with the wind velocity to avoid underestimating the concentrations.



347

Fig. 9. Comparison of the mean annual concentrations based on the "detailed" 18-velocity-range wind distribution using (A)the intermediate velocity and (B) the representative velocity.

350

351 *3.2.3. Continuous methodology using the sigmoid function*

For the last approach, mean annual concentrations based on CFD results can be calculated using a continuous methodology. This methodology is a combination of equation (4), describing the evolution of pollutant concentration with wind velocity, and equation (2), describing the evolution of wind velocity frequency with wind velocity. The equation to compute the mean annual concentrations continuously is given in (12).

357
$$\bar{C} = \frac{\int_0^{+\infty} c(v).f(v).dv}{\int_0^{+\infty} f(v).dv} + C_{bg} \quad (12)$$

where \bar{C} is the mean annual concentration, c(v) is the function describing the evolution of the concentration with the wind velocity, f(v) is the function describing the evolution of the wind velocity frequency with the wind velocity, and C_{bg} is the background concentration.

361 Taking equation (4) for c(v) and equation (2) for f(v) leads to a mathematical problem. Indeed,

362 c(v) is not defined for v = 0 and the limit of c(v). f(v) tends toward infinity when v tends

363 toward 0. To avoid this problem, equation (13) is suggested instead of equation (12). With this 364 equation, it is considered that a minimal velocity (v_{min}) exists for which the pollutant concentration will no longer increase when the wind velocity decreases. This hypothesis can be 365 366 justified by the additional effects, such as traffic-induced turbulence (Vachon et al., 2002) and 367 atmospheric stability (Qu et al., 2012) that may participate in pollutant dispersion for low wind 368 velocities or become preponderant. We suggest applying a constant pollutant concentration for wind velocities ranging from 0 to v_{min} and suggest using $C_{max} = c(v_{min})$. The choice of v_{min} 369 370 is particularly important when using the optimized sigmoid function.

371
$$\bar{C} = C_{max} \cdot \frac{\int_{0}^{v_{min}} f(v) \cdot dv}{\int_{0}^{+\infty} f(v) \cdot dv} + \frac{\int_{v_{min}}^{+\infty} c(v) \cdot f(v) \cdot dv}{\int_{0}^{+\infty} f(v) \cdot dv} + C_{bg} \quad (13)$$

where \bar{C} is the mean annual concentration, C_{max} is the maximal concentration accepted for the calculation, v_{min} is the velocity under which c(v) is considered equal to C_{max} , f(v) is equation (2), c(v) is equation (4) and C_{bg} is the background concentration.

Fig. 10. shows a comparison between the discrete methodology with the representative velocities and the continuous methodology using the optimized sigmoid function. It can be seen that the results of the discrete methodology given in Fig. 10. (A) can be reached by the continuous methodology. Nonetheless, the difference of 5% reached using $v_{min} = 0.01$ m/s can increase when changing the value of v_{min} : lower values will lead to higher concentrations whereas higher values will lead to lower concentrations. The value of v_{min} must therefore be chosen carefully.





Fig. 10. Comparison of the mean annual concentrations (A) based on the "detailed" 18-velocity-range wind distribution and using the intermediate velocity, and (B) based on the optimized sigmoid function and $v_{min} = 0.01$ m/s.

385 **4. Discussion**

This study provides tools to assess wind velocity distributions based on "basic" data and mean annual air pollutant concentrations based on CFD results. Additional work should be done to improve the methodologies and the major issues are discussed hereafter.

The capability of the Weibull and the sigmoid functions to describe wind velocity distribution 389 was assessed based on wind data from four meteorological stations in France. All of these 390 391 stations were located in peri-urban environments close to large French cities. It is necessary to 392 take into account that the results, and especially the interpolation-related errors, might be 393 different for other types of stations such as urban and rural stations, and for other countries with 394 different wind characteristics. In particular, the optimization suggested for the sigmoid function 395 may not be suitable for different countries or type of station. Further works are therefore 396 required in this direction.

397 The mean annual atmospheric pollutant concentrations can be calculated using a discrete 398 methodology. However, this methodology has two major problems. The first concerns the 399 choice of wind velocity for which the pollutant concentrations will be calculated: choosing an 400 intermediate velocity is a simple approach which can lead to considerable underestimations of 401 pollutant concentrations, and it is better to use a representative velocity instead, as suggested in 402 this paper. Using the representative velocity requires, however, making a choice for the first 403 velocity range. The second problem concerns the velocity step used to build the wind velocity 404 ranges: the result depends on the velocity step used, especially for the lower wind velocities for 405 which a decrease in the velocity-step leads to higher mean annual concentrations. To avoid 406 these two problems, a continuous methodology has been proposed. This methodology does not 407 have an intrinsic limitation, but dependent on the function describing the evolution of the 408 concentration as a function of wind velocity. If we consider a hyperbolic evolution of the 409 concentration with wind velocity, it is necessary to choose a minimal value of velocity for which it is considered that lower velocities will not increase the concentrations due to compensatory 410 411 phenomena (traffic-induced turbulence, atmospheric stability, etc.). The value of the minimal velocity is open to discussion and assessing this value is outside the scope of this paper. Further 412 works are required, for example with infield measurement campaigns and comparisons between 413 414 mean annual concentrations monitored and calculated with the continuous methodology.

Finally, it should be noted that the methodologies to assess mean annual concentrations were addressed using CFD results implying a neutral atmosphere, but can be used for any numerical results as long as a function describing the evolution of the concentration with the wind velocity is available.

419

420

421 **5. Conclusion**

422 The objectives of this study were to provide methodologies; (1) to assess wind velocity 423 distribution based on "basic" data, and (2) to assess mean annual air pollutant concentrations

- 424 based on numerical results. Three approaches for each objective were described and compared425 throughout this paper and the main conclusions are as follows:
- 426 (1.a) The Weibull distribution and the sigmoid function can both accurately reproduce
 427 "detailed" 18-velocity-range wind distribution based on "basic" 4-velocity-range wind
 428 data with an average error of 12%. These functions can nonetheless underestimate the
 429 frequencies of low velocities.
- 430 (1.b) The optimized sigmoid function improves the wind distribution results over the431 standard sigmoid function, especially for low wind velocities.
- (2.a) Using "basic" 4-velocity-range wind data and the discrete methodology can provide an
 estimation of the mean annual concentrations but is not sufficient to achieve high
 precision, leading to a difference of around 19% compared to the use of "detailed"
 18-velocity-range wind data. Using the sigmoid function instead, based on the "basic"
 wind data improves the mean annual concentration results with a global error of less
 than 4%.
- (2.b) When using the discrete methodology to assess mean annual concentrations, it is
 suggested to use a representative velocity of the function describing the evolution of
 pollutant concentrations with the wind velocities instead of an intermediate velocity.
 The intermediate velocity leads to underestimations of mean annual concentrations,
 especially when using CFD results with a neutral case hypothesis where the
 concentration evolves hyperbolically with the wind velocity.
- 444 (2.c) Mean annual concentrations can be assessed using a continuous methodology that does
 445 not have any of the limitations of discrete methodologies. It is, however, limited by
 446 the function describing the evolution of the concentrations with the wind velocities,
 447 which leads to the need to choose a minimal velocity when using the sigmoid function.

- 448 Finally, the methodologies presented in this paper can be used for outdoor air quality study
- 449 purposes, which is a relevant starting point for improving both outdoor and indoor air quality

450 and, therefore, a key-point to achieve smart sustainable cities.

451

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- 455

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